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Spin polarization of electrons beam in elastic scattering by carbon and oxygen atoms

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Abstract : The degree of spin polarizaton of an unpolarized electrons beam elastically scattered by carbon and oxygen atoms has been calculated in the static field polarization approximation over a wide incident energy range of 100-800 eV. In absence of any data or other theoretical calculations we employed three different approaches to calculate the degree of spin polarization for these atoms. We calculated direct scattering amplitude $f(\theta)$ all the times in the partial waves but the spin flip scattering amplitude $g(\theta)$ has been obtained, respectively, in first-Born, semi-classical approximation and in partial waves and the corresponding values of spin polarization are known as first-Born, semi-classical and partial-wave results. It is found that there are large differences in the three sets of values of spin polarization both qualitatively and quantitatively. The partial-wave values are always much higher than the values of the other two sets throughout the whole angular range and at all incident energies considered for both the atoms.

Keywords : Spin polarization, Born and semi-classical approximations, elastic scattering, electrons, static field polarization approximation

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The spin polarization effects in elastic scattering were predicted for the first time by Mott [1] who studied the scattering problem by Dirac equation. Since then all the calculations of spin polarization made use of Dirac equation in which spin-orbit interaction is most naturally included. These studies have been carried out for heavy atoms namely Ar,Kr,Xe,Au,Hg and Bi etc. The measurements of spin polarization parameters are however scarce and such measurements have not been carried out for about one and half decade after the prediction of Mott. Insight gained from the studies of heavy atoms leads to the question whether large values of spin polarization are to be expected in scattering of electrons by light atoms and whether the non-relativistic treatment of the problem may yield same results as obtained by the relativistic treatment in case of lighter atoms.

Some time ago McCarthy *et al* [2] and Lucas and McCarthy [3] carried out non-relativistic calculations of spin polarization for inert gases using optical potential approach and they got a disappointment when their results were compared with the then available experimental data of Schackert [4] and Kessler *et al* [5]. The agreement with the new data of Klewer *et al* [6] was also not satisfactory particularly below 150 eV. However, in a recent

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investigation by Khare and Raj [7] have found that a non-relativistic approach also yield same values of spin polarization as obtained by the relativistic one in case of ē-Ar elastic scattering.

To the best of our knowledge, no experimental data are available so far, on spin polarization for atoms lighter than Ne with an exception of He and only the relativistic calculations of Fink and Yates [8] carried out in static field, are available. Thus the situation which today exists for lighter atoms, is highly unsatisfactory as far as study of spin polarization in ē-atom elastic scattering is concerned. Hence, study of spin polarization of electrons by lighter atoms is not only interesting but important also. In the present investigation, we have solved the non-relativistic Schrödinger equation to obtain the degree of spin polarization for ē-C and ē-O elastic scattering over a wide incident energy range of 100-800 eV in static field polarization approximation. In absence of any data and other theoretical calculation, we have employed three different approaches *e.g.* first-Born, semiclassical and partial waves to calculate spin flip scattering amplitude $g(\theta)$ while the direct scattering amplitude $f(\theta)$ has been obtained in partial waves all the time. Corresponding results are termed as first-Born, semi-classical (SC) and particle wave (PW) results, respectively.

The spin polarization vector $P(\theta)$ of the unpolarized electron beam after scattering is given by [9]

$$P(\theta) = S(\theta)\hat{n} \tag{1}$$

where $S(\theta)$ is Sherman function which determines the degree of spin polarization and asymmetry if incident beam has initial transverse polarization. $\hat{n}$ is a unit vector perpendicular to the scattering plane. $S(\theta)$ is given by

$$S(\theta) = i\,\frac{f(\theta)g^*(\theta) - f^*(\theta)g(\theta)}{|f|^2 + |g|^2} \tag{2}$$

$f(\theta)$ and $g(\theta)$ are, respectively, direct and spin flip scattering amplitudes and in partial waves may be obtained from the following relations :

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}\left[(l+1)(e^{2i\delta_l^+} - 1) + l(e^{2i\delta_l^-} - 1)\right]p_l(\cos\theta) \tag{3}$$

$$g(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}\left(e^{2i\delta_l^-} - e^{2i\delta_l^+}\right)P_l^1(\cos\theta). \tag{4}$$

$\delta_l^{\pm}$ are the scattering phase shifts, respectively, for $J=l\pm1/2$. P_l $(\cos\theta)$ and P_l^1 $(\cos\theta)$ are ordinary and associated Legendre polynomials, respectively. k is the magnitude of the momentum vector of the incident electron. To obtain $\delta_l^{\pm}$, the non-relativistic Schrödinger equation was solved numerically under proper boundary conditions with an optical potential, $V_{op}(r)$. The optical potential is real and spherically symmetric. It includes the static [10], polarization [11] and the spin-orbit interaction potentials. The spin-orbit interaction, $V_{so}(r)$ is given by

$$V_{SO}(r) = \frac{\alpha^2}{2} \underline{l}.\underline{s} \frac{1}{r} \frac{dV_c(r)}{dr} \tag{5}$$

α is the fine-structure constant. $V_c(r)$ is a sum of static and polarization potentials. It may be noted that the static potential [10] used in the present investigation gives almost the same values of the spin polarization as obtained by Fink and Yates [8] through relativistic approach for C and O atoms.

It is evident from eq. (4) that $g(\theta)$ goes to zero in absence of spin orbit interaction since then $\delta_l^+ = \delta_l^- = \delta_l$. Furthermore, it may also be noted that the main contribution to the scattering amplitude from higher partial waves when $\delta_l^+ \simeq \delta_l^-$, comes through $f(\theta)$ only. We have taken the first few partial-wave phase-shifts ($l \leq 20$) exactly, and the contribution of all the higher remaining partial waves is included through the first-Born approximation in eq. (3). These values of $f(\theta)$ and $g(\theta)$ were used to calculate $S(\theta)$ and the corresponding results are termed as partial wave (PW) results.

In the second approach, $g(\theta)$ was calculated in the first-Born approximation for $V_{so}(r)$ [12] and $f(\theta)$ was calculated again in partial waves but taking $\delta_l^{\pm} = \delta_l$ $f(\theta)$ and $g(\theta)$ so calculated were used to obtain the values of $S(\theta)$ known as Born values. Lastly, we take

$$\delta_l^j \simeq \delta_l + \delta_{lso}^j \tag{6}$$

δ_{lso}^j are the phase shifts due to $V_{so}(r)$ calculated in semi-classical approximation [13]. The values of $\delta_l^{\pm}$ as given by eq. (6) were used to obtain the values of $f(\theta)$ and $g(\theta)$ and finally calculated $S(\theta)$. These values of $S(\theta)$ are known as semi-classical (SC) results. The present results are shown in Tables 1 and 2, respectively, for carbon and oxygen atoms.

For carbon atom (Table 1), we notice that Born and semi-classical approach predict a peak (maximum positive spin polarization) at 45° at 100 eV whereas partial wave method gives it at 50°. The positions of peaks and dips are underlined in the tables. The magnitude of the maximum in partial waves is about one and two-order higher, respectively, than that obtained in Born and semi-classical approaches. The dip (negative peak of spin polarization) is obtained at 100° in Born and at 105° in semi-classical approach with the order of magnitude same. However, in partial waves, the dip occurs at 100° (same as in Born approximation), but it is about two-orders of magnitude higher than that obtained in the other two approaches. At both 400 and 800 eV the peaks of spin polarization occur at 35° in partial waves. In Born approximation for an incident energy of 400 eV, the polarization peak occurs at 40° while for 800 eV, it occurs at 45°. No peak is obtained in the semi-classical approach after 100 eV. As the incident energy is increased from 100 eV to 800 eV, the position of dip is shifted to 160°, 110° and 120°, respectively, in first-Born, semi-classical and partial-wave approaches. Thus the shift of the dip is maximum (60°) in Born and least (5°) in semi-classical approach. For oxygen atom also (Table 2), we notice the same features as noted in case of carbon atom *i.e.* polarization peak is shifted to lower and dip to higher scattering angles as the incident energy increases. Furthermore, the magnitude of the peak or dip in partial waves is much larger than obtained in other two approaches. It may be noted that the above three approaches give almost same values for differential, integral and momentum transfer cross sections but the features of spin polarization are predicted differently. Further conclusions are not possible due to absence of any experimental data.

Table 1 Values of degree of spin polarization, $S(\theta)$ for $\bar{e}$ carbon elastic scattering at various impact energies.

Angle θ	100 eV Born	100 eV SC	100 eV PW	400 eV Born	400 eV SC	400 eV PW	800 eV Born	800 eV SC	800 eV PW
5	1.06–5	8.39–7	9.82–5	3.50–5	–6.51–7	1.73–4	5.52–5	–2.15–7	1.65–4
10	2.78–5	–2.45–7	3.24–4	8.56–5	–4.05–6	4.60–4	1.43–4	–6.80–6	4.41–4
15	5.12–5	–1.45–6	7.20–4	1.61–4	–7.49–6	9.50–4	3.03–4	–2.28–5	9.64–4
20	8.07–5	–3.93–7	1.20–3	2.63–4	–1.20–5	1.63–3	4.92–4	–2.80–5	1.62–3
25	1.15–4	3.26–6	1.70–3	3.75–4	–2.12–5	2.38–3	6.68–4	–4.12–5	2.42–3
30	1.53–4	7.59–6	2.36–3	4.78–4	–3.84–5	3.18–3	8.38–4	–9.97–5	3.66–3
35	1.91–4	1.07–5	3.28–3	5.45–4	–5.91–5	3.63–3	9.47–4	–1.32–4	4.25–3
40	2.22–4	1.24–5	4.27–3	5.72–4	–8.48–5	3.11–3	1.03–3	–1.39–4	2.61–3
45	2.40–4	1.31–5	5.20–3	5.61–4	–1.20–4	2.30–3	1.064–3	–2.13–4	1.45–3
50	2.37–4	1.00–5	6.01–3	5.19–4	–1.57–4	1.44–3	1.04–3	–2.82–4	2.54–3
55	2.09–4	–1.46–6	5.79–3	4.64–4	–1.91–4	–9.58–4	1.062–3	–2.92–4	1.03–3
60	1.58–4	–2.34–5	3.96–3	3.96–4	–2.30–4	–4.80–3	1.04–3	–3.45–4	–7.05–3
65	8.97–5	–5.35–5	1.54–3	3.15–4	–2.66–4	–8.09–3	9.31–4	–4.24–4	–1.34–2
70	1.64–5	–8.76–5	–1.46–3	2.35–4	–2.99–4	–1.14–2	8.76–4	–4.50–4	–1.66–2
75	–5.11–5	–1.22–4	–5.48–3	1.58–4	–3.31–4	–1.57–2	8.58–4	–4.82–4	–1.93–2
80	–1.05–4	–1.54–4	–8.82–3	8.12–5	–3.57–4	–1.97–2	7.23–4	–5.40–4	–2.72–2
85	–1.44–4	–1.80–4	–1.09–2	1.09–5	–3.78–4	–2.22–2	6.05–4	–5.66–4	–3.35–2
90	–1.67–4	–1.98–4	–1.31–2	–5.23–5	–3.98–4	–2.58–2	5.70–4	–5.90–4	–3.98–2
95	–1.768–4	–2.09–4	–1.54–2	–1.08–4	–4.10–4	–3.18–2	4.76–4	–6.21–4	–5.12–2
100	–1.769–4	–2.15–4	–1.61–2	–1.52–4	–4.14–4	–3.58–2	3.49–4	–6.18–4	–6.04–2
105	–1.70–4	–2.16–4	–1.52–2	–1.91–4	–4.18–4	–3.51–2	2.91–4	–6.29–4	–5.68–2
110	–1.59–4	–2.11–4	–1.37–2	–2.21–4	–4.17–4	–3.48–2	2.38–4	–6.50–4	–5.41–2
115	–1.46–4	–2.01–4	–1.21–2	–2.39–4	–4.05–4	–3.81–2	1.50–4	–6.17–4	–6.41–2
120	–1.31–4	–1.90–4	–1.08–2	–2.50–4	–3.92–4	–4.14–2	9.31–5	–5.91–4	–8.09–2
125	–1.16–4	–1.78–4	–1.05–2	–2.58–4	–3.79–4	–3.86–2	5.56–5	–6.03–4	–7.35–2
130	–1.02–4	–1.65–4	–1.10–2	–2.54–4	–3.54–4	–3.39–2	1.33–5	–5.62–4	–5.69–2
135	–8.84–5	–1.50–4	–1.12–2	–2.42–4	–3.27–4	–3.32–2	–1.57–5	–4.94–4	–5.60–2
140	–7.56–5	–1.33–4	–1.03–2	–2.31–4	–3.03–4	–3.58–2	–3.91–5	–4.81–4	–7.17–2
145	–6.38–5	–1.16–4	–8.49–3	–2.13–4	–2.71–4	–3.44–2	–5.68–5	–4.51–4	–7.45–2
150	–5.29–5	–1.00–4	–6.58–3	–1.87–4	–2.33–4	–2.64–2	–5.43–5	–3.62–4	–4.79–2
155	–4.27–5	–8.48–5	–5.28–3	–1.61–4	–2.00–4	–1.89–2	–5.52–5	–3.13–4	–3.42–2
160	–3.33–5	–6.83–5	–5.07–3	–1.34–4	–1.64–4	–1.51–2	–6.12–5	–2.81–4	–3.61–2

Format A±n means $A \times 10^{\pm n}$.

In conclusion, it may be stated that the various features of spin polarization (positions of peaks and dips and their magnitudes etc.) are predicted differently by the three different approaches employed in the present investigation. In a most recent investigation, Khare and Raj [7] found that the values of spin polarization obtained through present partial-wave approach are in good agreement with the other available theoretical calculations and the experimental data for $\bar{e}$-Ar elastic scattering. Hence, the present partial wave values of spin polarization for carbon and oxygen atoms are expected to be fairly reliable. For further conclusions, other theoretical investigations and experimental measurements of spin polarization for these atoms are highly desirable.

Table 2 Values of degree of spin polarization, $S(\theta)$ for $\bar{e}$-oxygen elastic scattering at various impact energies.

	100 eV			400 eV			800 eV		
Angle θ	Born	SC	PW	Born	SC	PW	Born	SC	PW
5	1.52–5	–8.25–7	–2.42–5	4.23–5	2.36–7	1.37–5	7.14–5	–6.91–7	1.50–4
10	3.58–5	–3.10–6	7.91–6	1.06–4	–3.67–6	8.69–5	1.77–4	–7.00–6	3.78–4
15	6.25–5	–5.45–6	1.83–4	1.92–4	–3.60–6	4.26–4	3.40–4	–1.39–5	7.52–4
20	9.57–5	–6.14–6	5.03–4	3.04–4	–1.88–6	1.23–3	5.51–4	–1.96–5	1.30–3
25	1.35–4	–3.90–6	8.89–4	4.34–4	–3.58–6	2.37–3	7.72–4	–3.39–5	2.10–3
30	1.78–4	1.74–6	1.42–3	5.64–4	–6.97–6	3.47–3	9.61–4	–6.73–5	3.17–3
35	2.20–4	1.10–5	2.34–3	6.61–4	–1.32–5	4.02–3	1.07–3	–1.04–4	3.81–3
40	2.53–4	2.45–5	3.62–3	7.00–4	–3.23–5	3.77–3	1.10–3	–1.47–4	3.11–3
45	2.69–4	4.30–5	5.09–3	6.71–4	–5.59–5	3.56–3	1.05–3	–2.15–4	2.16–3
50	2.58–4	6.47–5	6.74–3	5.82–4	–1.09–4	3.75–3	9.46–4	–2 85–4	1.72–3
55	2.16–4	8.42–5	8.19–3	4.53–4	–1.62–4	3.04–3	8.24–4	–3.50–4	2.85–4
60	1.42–4	9.37–5	8.77–3	3.03–4	–2.23–4	6.49–4	6.76–4	–4.26–4	–3.11–3
65	4.15–5	8.60–5	8.71–3	1 48–4	–2.85–4	–2.33–3	5.00–4	–4.98–4	–6.69–3
70	–7.35–5	5.56–5	7.62–3	1.22–6	–3.46–4	–5.68–3	3.34–4	–5.64–4	–1.06–2
75	–1.85–4	5.20–7	3.82–3	–1.31–4	–4.03–4	–9.32–3	1.75–4	–6.33–4	–1.54–2
80	–2.73–4	–7.45–5	–1.04–3	–2.44–4	–4.54–4	–1.20–2	1.73–5	–6.87–4	–1.92–2
85	–3.23–4	–1.56–4	–5.09–3	–3.36–4	–4.98–4	–1.40–2	–1.24–4	–7.29–4	–2.16–2
90	–3.31–4	–2.28–4	–9.67–3	–4.08–4	–5.35–4	–1.69–2	–2.54–4	–7.79–4	–2.55–2
95	–3.07–4	–2.78–4	–1.38–2	–4.59–4	–5.59–4	–2.08–2	–3.64–4	–8.08–4	–3.19–2
100	–2.65–4	–3.07–4	–1.53–2	–4.91–4	–5.74–4	–2.32–2	–4.45–4	–8.12–4	–3.61–2
105	–2.18–4	–3.16–4	–1.51–2	–5.07–4	–5.82–4	–2.30–2	–5.21–4	–8.29–4	–3.54–2
110	–1.72–4	–3.11–4	–1.43–2	–5.10–4	–5.80–4	–2.26–2	–5.83–4	–8.39–4	–3.56–2
115	–1.33–4	–2.96–4	–1.30–2	–5.01–4	–5.67–4	–2.28–2	–6.06–4	–8.11–4	–3.99–2
120	–1.00–4	–2.75–4	–1.14–2	–4.83–4	–5.51–4	–2.27–2	–6.20–4	–7.88–4	–4.33–2
125	–7.45–5	–2.51–4	–9.85–3	–4.58–4	–5.27–4	–2.18–2	–6.35–4	–7.72–4	–3.99–2
130	–5.46–5	–2.27–4	–8.37–3	–4.26–4	–4.94–4	–2.08–2	–6.17–4	–7.22–4	–3.53–2
135	–3.94–5	–2.02–4	–6.75–3	–3.91–4	–4.59–4	–1.96–2	–5.80–4	–6.63–4	–3.53–2
140	–2.80–5	–1.77–4	–5.23–3	–3.52–4	–4.21–4	–1.76–2	–5.52–4	–6.23–4	–3.75–2
145	–1.96–5	–1.52–4	–4.01–3	–3.11–4	–3.74–4	–1.47–2	–5.10–4	–5.60–4	–3.44–2
150	–1.34–5	–1.29–4	–2.98–3	–2.68–4	–3.25–4	–1.18–2	–4.42–4	–4.76–4	–2.70–2
155	–8.95–6	–1.06–4	–2.06–3	–2.24–4	–2.78–4	–9.82–3	–3.79–4	–4.13–4	–2.16–2
160	–5.81–6	–8.42–5	–1.38–3	–1.80–4	–2.24–4	–9.36–3	–3.19–4	–3.44–4	–1.90–2

Format A±n means $A \times 10^{\pm n}$.

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